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Assessment of a Molecular Diffusion Model in MELCOR

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INTRODUCTION

The MELCOR (version 1.8.5) [1] computer code with INEEL revisions is being improved for the analysis of very high temperature gas-cooled reactors [2]. Following a loss-of-coolant accident, flow through the reactor vessel may initially stagnate due to a non-uniform concentration of helium and air. However, molecular diffusion will eventually result in a uniform concentration of air and helium. The differences in fluid temperatures within the reactor vessel will then result in the establishment of a natural circulation flow that can supply significant amounts of air to the reactor core. The heat released by the resulting oxidation of graphite in the reactor core has the potential to increase the peak fuel temperature. In order to analyze the effects of oxidation on the response of the reactor during accidents, a molecular diffusion model was added to MELCOR. The model is based on Fick's Second Law for spatially uniform pressure and temperature. This paper describes equimolal counter diffusion experiments in a two bulb diffusion cell and the results of the assessment calculations.

EXPERIMENT DESCRIPTION

Two validate the diffusion model added to the MELCOR code the diffusion of a ternary gas mixture corresponding to the experiment described by Duncan and Toor [3] was used. A schematic of Duncan and Toor experiment is shown in Figure 1. The experiment consisted of two volumes connected by a short capillary diffusion line. The two volumes are referred to in the figure as Bulb #1 and Bulb #2. Bulbs #1 and #2 have volumes of 77.99 cm^3 and 78.63 cm^3, respectively. The diffusion line connecting the two bulbs was 85.9 mm long with an internal diameter of 2.08 mm. The diffusion line contained a stopcock, which was used to separate the gas mixture contained in bulb #1 from the gas mixture contained in bulb #2. The gas contained in bulb #1 was a mixture of nitrogen and carbon dioxide with a molar composition of 50.086 percent nitrogen and 49.914 percent carbon dioxide. The gas mixture in bulb #2 contained nitrogen and hydrogen with a molar composition of 49.879 percent nitrogen and 50.121 percent hydrogen. When thermal (32.5°C) and mechanical (1 atm) equilibrium was established between the two bulbs, the stopcock was opened allowing the diffusion process to begin.

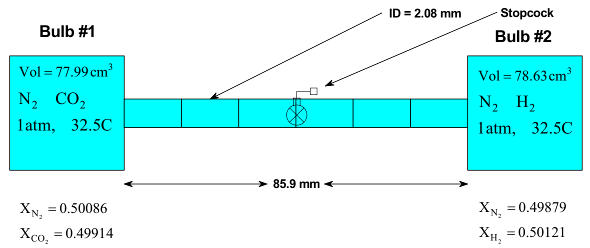

Figure 1. Schematic of the two-bulb experiment.

At the end of the run the stopcock was closed and the contents of the bulbs were analyzed by gas chromatography.

RESULTS

The results from the experiment show that the nitrogen in bulb #2, which has a slightly higher concentration of N_2, begins to diffuse toward bulb #1. In a short time (≈ 130 sec) the mole fraction of N_2 in bulb #2 drop below the mole fraction of N_2 in bulb #1, however the mole fraction of N_2 in bulb #2 continues to decrease while the mole fraction of N_2 in bulb #1 increases. This trend continues until approximately 6 hr at which time the mole fraction in bulb #1 stops increasing and starts to decrease. At this time the mole fraction in bulb #2 stops decreasing and starts to increase. The period between 130 sec and 6 hr is referred to as the reverse diffusion of nitrogen.

CONCLUSIONS

From this study, we conclude that the MELCOR results compare very well with the experimental results for the diffusion of a ternary gas mixture. We will continue to perform more comparison studies using other data.

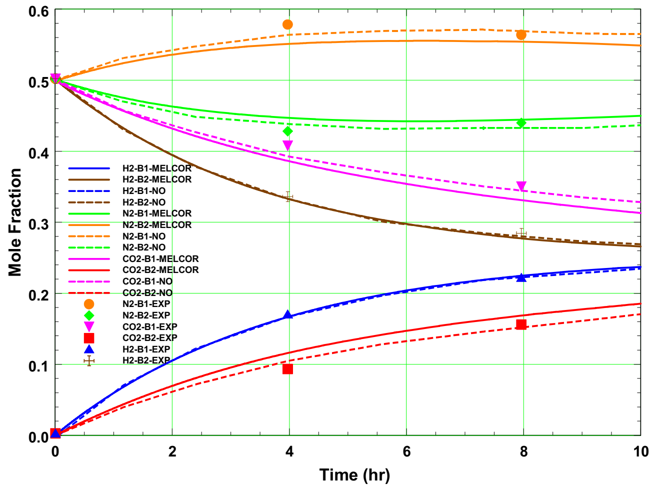

Figure 2. Multi-component diffusion results.

ACKNOWLEDGMENT

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3. J.B. Duncan and H.L. Toor, "An Experimental Study of Three Component Gas Diffusion," *AIChE J.*, March, 1962, pp. 38-41.